

Emergence of U(1) symmetry in the 3D XY model with Z_q anisotropy

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We study the three-dimensional XY model with a Z_q anisotropic term. At temperatures $T < T_c$ this dangerously irrelevant perturbation is relevant only above a length scale Λ , which diverges as a power of the correlation length; $\Lambda \sim \xi^{a_q}$. Below Λ the order parameter is U(1) symmetric. We derive the full scaling function controlling the emergence of U(1) symmetry and use Monte Carlo results to extract the exponent a_q for $q = 4, \dots, 8$. We find that $a_q \approx a_4(q/4)^2$, with a_4 only marginally larger than 1. We discuss these results in the context of U(1) symmetry at “deconfined” quantum critical points separating antiferromagnetic and valence-bond-solid states in quantum spin systems.

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A salient feature of the recently proposed theory of “deconfined” quantum critical points, which separate Néel and valence-bond-solid (VBS) ground states of antiferromagnets on the square lattice, is the emergence of U(1) symmetry [1]. The VBS is either dimerized on columns or forms a square pattern with plaquettes of four strongly entangled spins [2, 3]. In both cases there are four degenerate patterns and, thus, Z_4 symmetry is broken. However, as the critical point is approached the theory predicts a length scale Λ , diverging faster than the correlation length, $\Lambda \sim \xi^a$, $a > 1$, below which the distinction between columnar and plaquette VBS states disappears. The nature of the VBS state is manifested only when coarse-graining on length-scales $l > \Lambda$, whereas for $l < \Lambda$ the Z_4 symmetry is unbroken and is replaced by an emergent U(1) symmetry characterizing the fluctuations between columnar and plaquette order.

Quantum Monte Carlo simulations [4] of an $S = 1/2$ Heisenberg model with four-spin couplings have recently provided concrete evidence for a continuous Néel–VBS transition, and also detected U(1) symmetry in the VBS order-parameter distribution $P(D_x, D_y)$, where D_x and D_y are VBS order parameters for horizontal and vertical dimers. There is no trace of the expected Z_4 anisotropy in the VBS phase—the distribution is ring shaped—although the finite-size scaling of the squared order parameter shows that the system is long-range ordered. This can be interpreted as the largest studied lattice size $L = 32 < \Lambda$. A ring-shaped distribution was also found in simulations of an $SU(N)$ generalization of the $S = 1/2$ Heisenberg model [5]—possibly a consequence of proximity of this system to a deconfined quantum-critical point.

In order to better understand the U(1) features of these VBS states, and to guide future studies of them, we here exploit a classical analogy. In the three-dimensional XY model including a Z_q -anisotropic term,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - h \sum_i \cos(q\theta_i), \quad (1)$$

the anisotropy is dangerously irrelevant for $q \geq 4$ [6, 7, 8,

9, 10], i.e., the universality class is that of the isotropic XY model but the perturbation is relevant for $T < T_c$ above a length-scale Λ . In the closely related q -state clock model, the anisotropy is dangerously irrelevant for $q \geq 5$. While numerical studies [11, 12, 13] have confirmed the irrelevance of the anisotropy at T_c , the associated Λ has, to our knowledge, not been extracted numerically, except for an analysis of the 3-state antiferromagnetic Potts model, which corresponds to Z_6 [9, 14].

Here we report results of Monte Carlo simulations for $4 \leq q \leq 8$ on periodic-boundary lattices with $N = L^3$ sites and L up to 32. In addition to Metropolis single-spin updates, we also use Wolff cluster updates [15] to reduce critical slowing down. We sample the order-parameter distribution $P(m_x, m_y)$, where

$$m_x = \frac{1}{N} \sum_{i=1}^N \cos(\theta_i), \quad m_y = \frac{1}{N} \sum_{i=1}^N \sin(\theta_i). \quad (2)$$

The standard order parameter can be defined as

$$\begin{aligned} \langle m \rangle &= \int_{-1}^1 dm_x \int_{-1}^1 dm_y P(m_x, m_y) (m_x^2 + m_y^2)^{1/2} \\ &= \int_0^1 dr \int_0^{2\pi} d\theta r^2 P(r, \theta). \end{aligned} \quad (3)$$

We will compare this with an order parameter $\langle m_q \rangle$ which is sensitive to the angular distribution;

$$\langle m_q \rangle = \int_0^1 dr \int_0^{2\pi} d\theta r^2 P(r, \theta) \cos(q\theta). \quad (4)$$

While the finite-size scaling of $\langle m \rangle$ is governed by the correlation length ξ , $\langle m_q \rangle$ should instead be controlled by the U(1) length scale Λ [9], becoming large for a system of size L only when $L > \Lambda$. Fig. 1 shows magnetization histograms at $h/J = 1$ for Z_4 and Z_8 systems with $L = 4$ and 32. The angular distribution $P(\theta) = \int dr r P(r, \theta)$ is also shown. The average radius of the distribution is the magnetization $\langle m \rangle$, which decreases with increasing L . The anisotropy, on the other hand, increases with

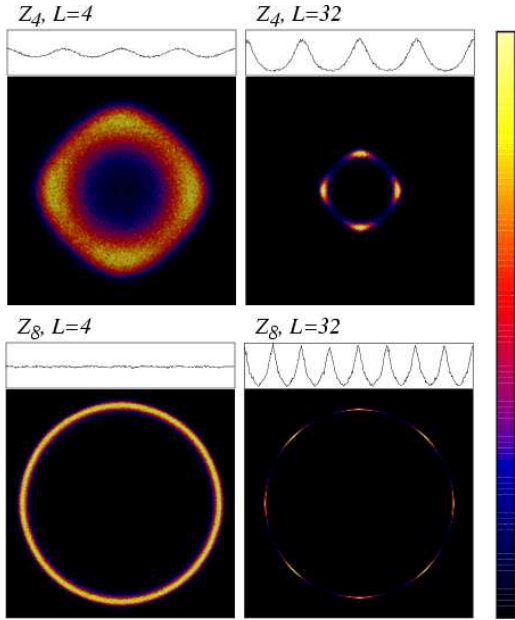


FIG. 1: (Color online) $P(m_x, m_y)$ at $h/J = 1$ for $q = 4, 8$, $L = 4, 32$. The temperature $T/J = 2.17$ for Z_4 and 1.15 for Z_8 ; both less than $T_c/J \approx 2.20$. The size of the histograms corresponds to $m_{x,y} \in [-1, 1]$. Angular distributions $P(\theta)$ with $\theta \in [0, 2\pi]$ are shown above each histogram.

L . This is particularly striking for Z_8 , where the $L = 4$ histogram shows essentially no angular dependence, even though T is very significantly below T_c , whereas there are 8 prominent peaks for $L = 32$. Thus, in this case the $U(1)$ length scale $4 < \Lambda < 32$. For the Z_4 system T is much closer to T_c but still some anisotropy is seen for $L = 4$; it becomes much more pronounced for $L = 32$.

It is instructive to examine a spin configuration with $m_x \approx m_y$, i.e., $\theta \approx \pi/4$. Fig. 2 shows one layer of a Z_4 system with $L = 10$ below T_c . The spins align predominantly along $\theta = 0$ and $\theta = \pi/2$, with only a few spins in the other two directions. Clearly there is some clustering of spins pointing in the same direction—the system consists of two interpenetrating clusters. Essentially, the configuration corresponds to a size-limited domain wall between $\theta = 0$ and $\theta = \pi/4$ magnetized states.

Hove and Sudbø studied the q -state clock model and performed a course graining at criticality [13]. They found that the structure in the angular distribution diminished with the size of the block spins for $q \geq 5$, as would be expected if the anisotropy is irrelevant. Here we want to quantify the length scale Λ at which the anisotropy becomes relevant for $T < T_c$. Consider first what would happen in a course graining procedure for a single spin configuration of an infinite system in the ordered state very close to T_c . The individual spins will of course exhibit q preferred directions, as is seen clearly in Fig. 2, i.e., there would be q peaks in the probability distribution of angles θ_i . Constructing block spins of l^3 spins, we would expect the angular dependence to first

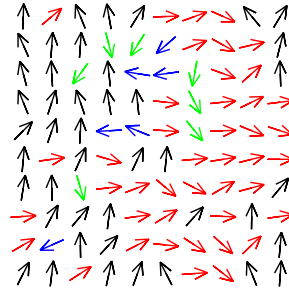


FIG. 2: (Color online) Spins in one layer of the Z_4 model with $L = 10$ at $h/J = 1, T/J = 1.9 < T_c$. Here $m_x \approx m_y$, corresponding to $\theta \approx \pi/4$ in $P(r, \theta)$. Arrows are color-coded according to the closest Z_4 angle; $n\pi/2$, $n = 0, 1, 2, 3$.

become less pronounced because of the averaging over spins pointing in different directions (again, as is seen in Fig. 2). Sufficiently close to T_c we would expect the distribution to approach flatness. However, since we are in an ordered state, one of the q preferred angles eventually has to become predominant, and thus one peak in the histogram will start to grow. This happens at $l \approx \Lambda$. We cannot simulate the infinite system and instead we carry out an analogous procedure as a function of the lattice size L , sampling a large number of configurations. We calculate the order parameters $\langle m \rangle$ and $\langle m_q \rangle$, defined in Eqs. (3,4), and analyze them using

$$\langle m \rangle = L^{-\sigma} f(tL^{1/\nu}), \quad (5)$$

$$\langle m_q \rangle = L^{-\sigma} g(tL^{1/\nu_q}). \quad (6)$$

Here (5) is the standard finite-size ansatz with $\sigma = \beta/\nu$, and the XY exponents are $\beta \approx 0.348$ and $\nu \approx 0.672$ [17]. Eq. (6) is an intuitive generalization of (5), which was proposed and used also in Ref. [9], but we can actually also derive the scaling function $g(X)$ exactly.

Let us consider the scaling behavior of the order-parameter distribution $P(\vec{m})$. It depends upon the system size L and the size of scaling operators that perturb the critical theory. Specifically, we consider the temperature deviation $t = T_c - T$ and the presumed irrelevant q -fold anisotropy strength h . By conventional scaling arguments, we expect

$$P(\vec{m}; L, t, h) = L^{\sigma/2} \hat{P}(L^\sigma \vec{m}, tL^{1/\nu}, H = hL^{3-\Delta_q}), \quad (7)$$

where $\Delta_q > 3$ is the scaling dimension of the irrelevant anisotropy. The prefactor above is determined from normalization of the probability distribution. In the scaling regime, $|t| \ll 1, L \gg 1$, so H is small. When the first two arguments are $O(1)$, \hat{P} can be well-approximated by taking $H = 0$ [with “corrections to scaling” of $O(H)$, i.e. suppressed by $L^{3-\Delta_q}$ for a large system]. At $H = 0$, the distribution is fully XY symmetric, and the integral in Eq. (4) vanishes. Thus, in this regime $\langle m_q \rangle$ is small, $O(H)$, and should be considered as arising from corrections to scaling. This simply reflects the irrelevance of the anisotropy at the critical point.

Because the anisotropy is *dangerously* irrelevant, a larger contribution, however, emerges when $tL^{1/\nu} \gg 1$, i.e. $L \gg \xi \sim t^{-\nu}$. In this limit, the system can be regarded as possessing long-range XY order, and the only significant fluctuations are the *global* fluctuations of the XY phase θ . This is biased by the anisotropy. The scale κ of the total anisotropy (free) energy can be estimated by its typical magnitude within an XY correlation volume, $h\xi^{3-\Delta_q}$, multiplied by the number of correlation volumes, $(L/\xi)^3$, i.e. $\kappa = hL^3\xi^{-\Delta_q}$. Note that although the energy per correlation volume is small (due to the irrelevance of anisotropy at the critical point), the number of correlation volumes becomes very large and more than compensates for this smallness for L/ξ sufficiently large.

From this argument, we see that for $L/\xi \gg 1$, the distribution of angles θ is just determined from a Boltzmann factor for a single XY spin with the q -fold anisotropy energy $\sim -\kappa \cos q\theta$. Furthermore, for $L/\xi \gg 1$, the magnitude $|\vec{m}| \approx \langle m \rangle$ is approximately non-fluctuating. Thus the distribution factors into the form $P(|m|, \theta) = \langle m \rangle^{-2} \delta(|m| - \langle m \rangle) P(\theta)$, with

$$P(\theta) = \frac{1}{Z} e^{\kappa \cos(q\theta)}. \quad (8)$$

Here $Z = \int_0^{2\pi} d\theta e^{\kappa \cos(q\theta)}$ is the single-spin partition function. It is then straightforward to obtain from Eq. (4)

$$\langle m_q \rangle = \langle m \rangle \frac{I_1(\kappa)}{I_0(\kappa)}, \quad (9)$$

where I_n is the modified Bessel function of order n . Oshikawa obtained a similar expression in a different way, but we disagree with his scaling variable. Comparing this with the scaling form in Eq. (6), we see that $\nu_q = \Delta_q \nu / 3$ ($a_q = \Delta_q / 3$), $\kappa = h(tL^{1/\nu_q})^{3\nu_q}$, and

$$g(X) \propto \frac{I_1(\tilde{h}X^{3\nu_q})}{I_0(\tilde{h}X^{3\nu_q})}. \quad (10)$$

Here \tilde{h} should be viewed as a non-universal scale factor. From the above discussion, one sees that this form is valid for $L/\xi \gg 1$ but L/ξ_q arbitrary. For L/ξ of $O(1)$ or smaller, $L/\xi_q \ll 1$ (implying $\kappa, X \ll 1$), and the scaling form for $\langle m_q \rangle$ becomes small and of order the expected correction to scaling in the critical regime.

In Fig. 3 we show results for the two order parameters for systems with $q = 4, 5, 6$. We have studied several values of h/J and here show results for a different value for each q . We have extracted T_c using finite-size scaling of $\langle m \rangle$ with Eq. (5) and the XY exponents. This works very well for all q , confirming the irrelevance of h . The magnetization for $T < T_c$ is seen to decrease marginally with increasing q in Fig. 3. The Z_q order-parameter $\langle m_q \rangle$ changes more drastically, being strongly suppressed close to T_c for large q . This is expected, as $\langle m_q \rangle$ should vanish for all T in the XY limit $q \rightarrow \infty$. For Z_4 , the $\langle m_q \rangle$

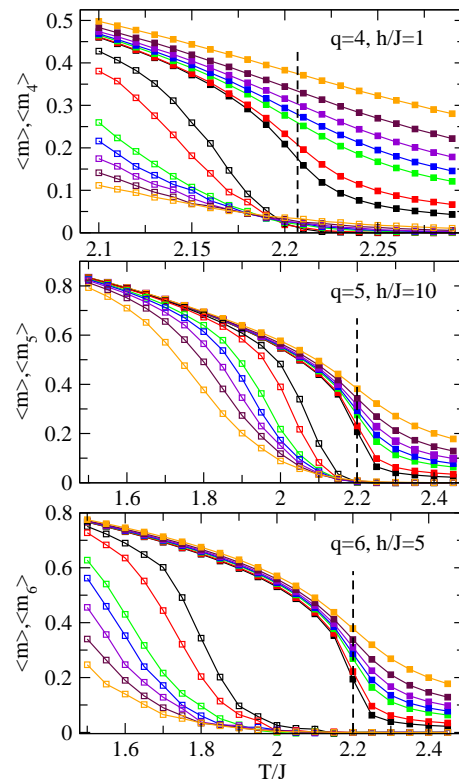


FIG. 3: (Color online) The XY order parameter $\langle m \rangle$ (solid curves) and the Z_q order parameter $\langle m_q \rangle$ (dashed curves) vs temperature for $q = 4, 5, 6$. The system sizes are $L = 8, 10, 12, 14, 16, 24$, and 32 . The curves become sharper (increasing slope) around T_c (indicated by vertical lines). The ratios h/J used are indicated on the graphs.

curves for different L cross each other, with the crossing points moving closer to T_c as L increases. This is consistent with the above discussion of course-graining: In the ordered state close to T_c , $\langle m_q \rangle$ should first, for small L , decrease with increasing L as the q -peaked structure in $P(\theta)$ diminishes due to averaging over more spins. For larger L , $\langle m_q \rangle$ starts to grow with L as the length-scale Λ is exceeded. This behavior is more difficult to observe directly for $q = 5, 6$ because $\langle m_q \rangle$ is small and dominated by statistical noise close to T_c where the curves cross.

Fig. 4 shows finite-size scaling of the Z_q order-parameter $\langle m_q \rangle$, using the hypothesis (6) and the XY value for σ . Adjusting $\nu_q = a_q \nu$ for each q we find satisfactory data collapse using $a_4 = 1.07(3)$, $a_5 = 1.6(1)$, $a_6 = 2.4(1)$, and, not shown in the figure, $a_8 = 4.2(3)$. These results are consistent with the form $a_q = a_4(q/4)^2$, in qualitative agreement with the ϵ -expansion by Oshikawa, which gave $a_q \rightarrow q^2/30$ for large q [9]. However, in the ϵ -expansion there are significant deviations from the q^2 form in the range of q values considered here. Our a_6 is also smaller than the value ≈ 3.5 obtained on the basis of the 3-state Potts antiferromagnet [9].

In Fig. 4 we also show the scaling function (10). It does not match exactly the collapsed data, but the agreement

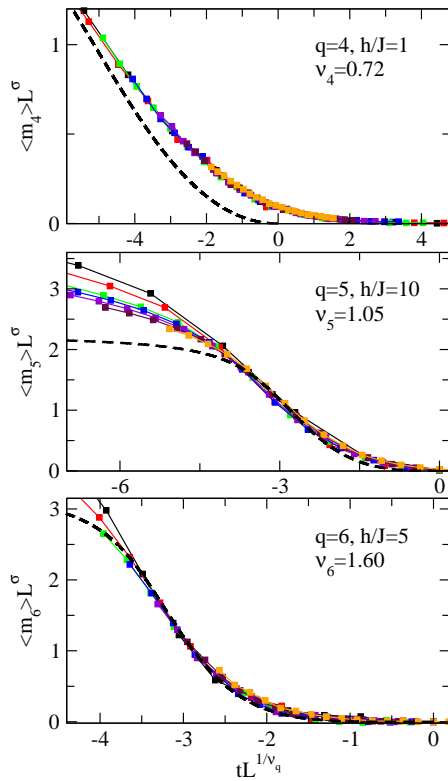


FIG. 4: (Color online) Scaling of the Z_q magnetization. We use $\sigma = 0.52$ for all q , and ν_q as indicated in the plots. The colors of the curves correspond to L as in Fig. 3. The dashed curves are the predicted scaling functions with \tilde{h} and prefactors adjusted to fit the data approximately.

improves as q increases. As we have discussed above, the scaling function represents the dominant behavior for $T < T_c$, but exactly at T_c this contribution vanishes and the critical-point scaling form $\langle m_q(T_c) \rangle \sim L^{3-\Delta_q}$ becomes dominant. For $q = 4$, $\Delta_4 - 3$ is small; our estimate is $\Delta_4 - 3 = 0.21(9)$, in good agreement with previous estimates of the scaling dimension [8, 10]. Thus it is clear that very large systems would be required for this contribution to become invisible on the scale used in our graph. It is also clear that for $t < 0$, close to $t = 0$, there will be a similarly significant correction to the asymptotically dominant scaling function. As q increases, we have seen that $\Delta_q = 3a_q$ increases rapidly, and we thus expect significantly smaller correction to scaling. For $q = 6$ the agreement is already seen to be quite good, considering that our lattices are not very large.

To conclude, we relate our results to the quantum VBS states discussed in the introduction. Returning to Fig. 2, associating $\theta_i \approx 0$ arrows with two adjacent horizontal dimers on even-numbered columns and $\theta_i \approx \pi/2$ with vertical adjacent dimers on even rows, $\langle \theta \rangle = 0, \pi/2$ correspond to columnar VBS states. A plaquette is a superposition of horizontal and vertical dimer pairs, whence a plaquette VBS corresponds to $\langle \theta \rangle = \pi/4$ [3]. Rotating the arrows by 90° corresponds to translating or rotating

a VBS. Either a columnar or plaquette VBS should obtain in the infinite-size limit, but close to a deconfined quantum-critical point, for $L < \Lambda$, the system fluctuates among all mixtures of plaquette and columnar states. This corresponds to a ring-shaped VBS order-parameter histogram. In numerical studies of quantum antiferromagnets [4, 5] no 4-peak structure was observed in the angular distribution, and hence it is not clear what type of VBS finally will emerge (although a method using open boundaries favors a columnar state in [4]). It seems unlikely that the $U(1)$ symmetry should persist as $L \rightarrow \infty$. In the classical Z_4 model we never observe a perfectly $U(1)$ -symmetric histograms far inside the ordered phase, in contrast to Refs. [4, 5]. On the other hand, a_q is larger for $q > 4$, and in Fig. 1 we have shown a prominently $U(1)$ -symmetric histogram for the Z_8 model deep inside the ordered phase. Thus, the exponent a may be larger for the Z_4 quantum VBS than $a_4 \approx 1$ obtained here for the classical Z_4 model. There is of course no reason to expect them to be the same, as the universality class of deconfined quantum-criticality is not that of the classical Z_4 model [1, 4]. Future numerical studies of VBS states and deconfined quantum-criticality can hopefully reach sufficiently large lattices to extract the $U(1)$ exponent using the scaling method employed here.

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